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Synthesis of a new quaternary phosphonium salt: NMR study of the conformational structure and dynamics

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Abstract

© 2015 John Wiley & Sons, Ltd. A novel phosphonium salt based on pyridoxine was synthesized. Conformational analysis of the compound in solution was performed using dynamic NMR experiments and calculations. The obtained results revealed some differences in the conformational transitions and the energy parameters of the conformational exchange of the studied compound in comparison to previously reported data for other phosphorus-containing pyridoxine derivatives. It was shown that increasing the substituent at the C-11 carbon leads to greater differences in the populations of stable states and the corresponding equilibrium energies.

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Keywords

Conformational transition, Dynamic 1H NMR, Energy barrier, Nuclear Overhauser effect, Quaternary phosphonium salts